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The Bound Polaron in Two Dimensions

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Dedication

I dedicate this work
to my
parents,
wonderful wife
and all my friends.

Acknowledgment

I am indebted to some who have encouraged me along the way and helped open doors for me.

I gratefully acknowledge the patience and support of

my supervisor

Dr.Bassam Saqqa

Abstract

The problem of a two dimensional bound polaron is studied using the adiabatic strong coupling approach. The energy, the number of phonons around the electron, and the size of the polaron are calculated for the ground and for the first two excited states. The effect of an external magnetic field on the problem is also investigated. It is observed that the three fields affect each other in an involved and interrelated manner. In the absence of the magnetic field it is found that the degeneracy of the two excited states is lifted at lower values of α as β decreases.

Arabic Abstract

باستخدام الطريقة الأديباتية، تم دراسة البولارون المحصور ثنائي الأبعاد حيث تم حساب الطاقة وعدد الفونونات المحيطة بالإلكترون وكذلك حجم البولارون للمستوى الأرضي والمستويين المثارين الأول والثاني. كما أن تأثير المجال المغناطيسي على المسأله تم دراسته أيضاً. لقد وجد أن شدة المجالات الثلاثة تؤثر على بعضها البعض بصورة ضمنية ومترابطة. بدون تأثر المجال المغناطيسي لوحظ أن ظاهرة الانحلال بين المستويين المثارين ترفع عند قيم أقل للثابت البولاروني α وذلك بنقصان ثابت كولوم β .

Chapter 1
Introduction

1.1 The Polaron Concept

An ideal crystal is constructed by the infinite repetition of identical structure units in space. In the simplest crystals, the structural unit is a single atom as in copper, silver, gold and alkali metals. But the smallest structural unit may comprise many atoms or molecules, the structure of all crystals can be described in terms of a lattice, with a group of atoms attached to every lattice point.

The atoms in a crystal located on sites called *lattice points*, at room temperature, these atoms are not fixed but rather vibrate about these points.

The displacement of any point of an elastic medium from the equilibrium position forms a vector field called *displacement field*. It is possible to quantize this field, the field quanta being known as *a phonon*.

An electron in a crystal can creats a displacement field around itself due to interaction between the electron and the ions forming the crystal. These phonons carry the energy and the momentum of the wave, the combination of the electron and the cloud of phonons is known as polaron.

The polaron concept is of interset, not only because it describes the particular physical properties of an electron in polar crystals and ionic semiconductors but also because it is an interesting theoretical model consisting of a fermion interacting with a scalar boson field.

The early work on polarons was concerned with general theoretical formulations and approximations, which now constitute the standard theory and with experiments on cyclotron resonance and transport properties [1] Now let us take the ionic crystal (KCl) of an impurity which is one of the causes of the conduction electron. Thus phonons of the two (K) ions interact with the conduction electron to give a polaron as shown in figure (1.1) below[2]:

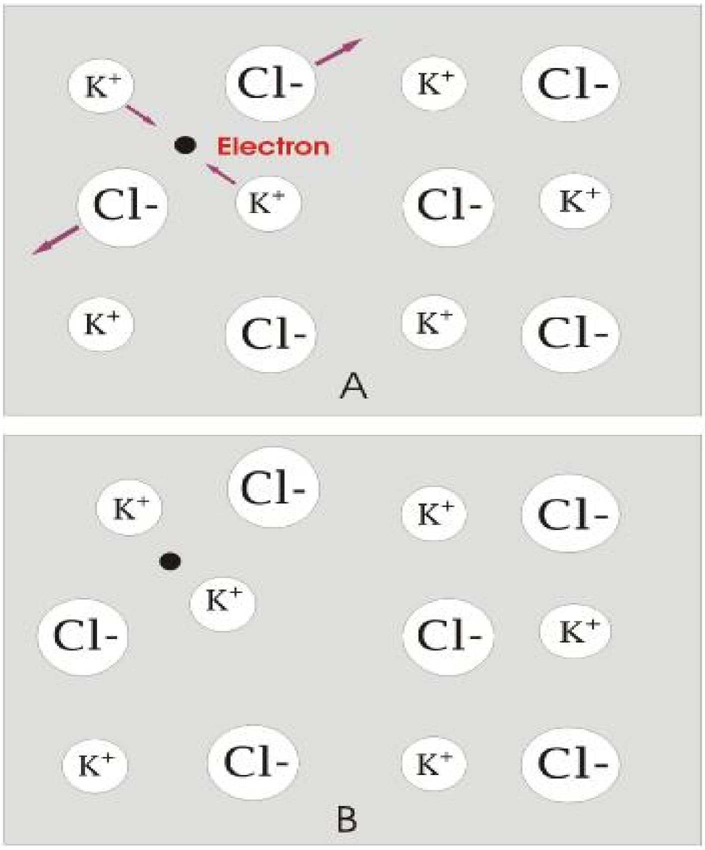

Figure 1.1 : The formation of a polaron. **A)** A conducting electron is shown in a rigid lattice of an ionic crystal, KCl. The force of the ions adjacent to the electron are shown . **B)** The electron is shown in an elastic or deformable lattice, the electron plus the associated strain field is called ***a polaron***.

For more understanding, let us take one of the simplest classical pictures of a polaron, consider a muscate on a soft surface of a jelly cake, by its weight the muscate deforms the surface of the jelly cake. If one gently pushes the muscate (on the jelly cake) it rolls away accompained by the deformation underneath as the one stil push it. In a solid state the conduction electron plays the role of the muscate and the ionic crystal plays the role of the jelly cake as shown in figure (1.2):

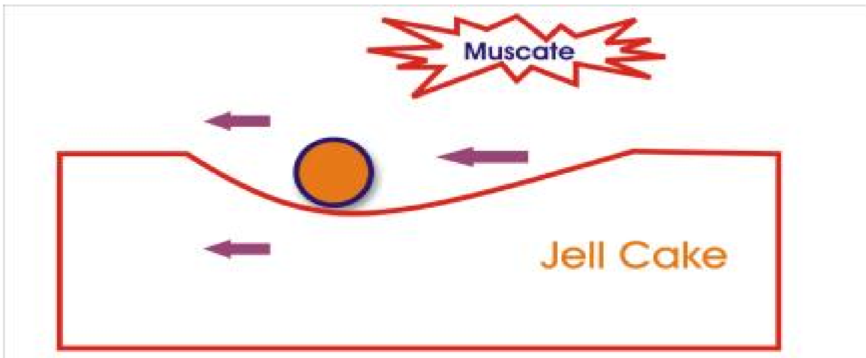

Figure 1.2 : An example describing the electron polarizes the medium that deforms and trap it.

1.2 Types of the Polaron

The polaron can be classified according to its size (*large* or *small*). *The small polaron* is formed when an electron is trapped by itself–induced atomic displacement field in a region of dimensions in the order of the lattice constant, or we can say that the deformation of the lattice is small.

On the other hand when the displacement of the ions are larger than the lattice constant, *a large polaron* is formed and the deformation of the lattice is large. The large polaron differs from the the small polaron in many aspects. In *large polaron* regime the lattice can be repalced by a continuum, disregarding the discreteness of the atoms at the lattice point, which is not appropriate for the *small polaron* regime. The effective mass of the *small polaron* is large enough to drastically altering the transport properties of the crystal, while the *large polaron* has a much smaller mass which is slightly larger than that of the bare bond electron.

There are many other types of polarons intermediate between the two extremes. Polarons can bind in pairs, the interaction of two electrons (or holes) with the phonon field may result into a composite quasiparticle called bipolaron. Bipolaronic effects are used in studing many materials like transition metal-oxides[3-6], polymers[7] and superconducting materials[8]. Bipolaron issue is assumed to be responsible for the formation of the pairing system in the high- T_c superconductivity, where

T_c is the critical temperature for the superconductivity phenomena[9], so it represents a good explanation for the theory of Bardeen, Cooper and Schrieffer(BCS) at (1957), and the bipolaron here called cooper pair.

1.3 Solving the polaron problem

The problem of an electron interacting with a crystal has been of interest since solid state physics began to develop in the early *1930* s where landau (*1933*) first introduced the concept of polaron. In *1937*, Fröhlich gave a quantitative discussion of electron scattering in ionic crystals where he introduced the concept of the field of the lattice displacement.

Later *1949* he derived the so-called "Fröhlich Hamiltonian" and solved the problem for the weak coupling case with perturbation theory. In *1953*,Lee,Low and pines (LLP)[10] developed a variational technique for intermediate coupling strengths by introducing a canonical transformation which enable one to handle the problem in a new frame of reference with the origin attached to the position of the electron.

In *1954* Pekar[11] developed the strong coupling theory, this theory is valid when the electrons kinetic energy in the potential well is much greater than the energy of the phonons contributing to the deformation.

Among all the approaches Feynmans path integral technique [12-16] considered to be the most powerful valid for all range of the coupling strengths. Feynmans method replaces the actual polaron by a system of two particles, the electron and a fictitions mass which takes the effect of the polarization field into accound in harmonic interaction.

In the last four decades, and due to the development achieved in modern fabrication techniques like moleculer beam epitaxy and metal organic-chemical vapour deposition, it has become possible to grow low dimensional superstructures opening a large area of research on two,one, and zero dimensional polarons. Of particular interset are the strict two-dimensional (2D) models accounting for the almost two-dimensional aspect of an electron in a thin quantum well and get interacting with the bulk LO(Longitudinal Optical) phonon modes (Das Sarma ,et al)[17]. The common finding along these lines is that the electron interacts more effectively with the phonons in two dimensions and consequently certain polaron quantities scale by considerably large factors over their corresponding bulk values. The polaron self energy, for instance, is inhanced by a factor of $\frac{p}{2}$ at weak coupling, and by $\frac{3p^2}{8}$ under the strong coupling regime. Similar features show up for further other quantities like the effective polarons mass or the mean number of phonons clothing the

electron (table 1.1). Going on further to confinement geometrices of lower dimensionalities, like the one-dimensional wire and even zero-dimensional quantum box, the binding energy can be made much stronger than for the 3-D and 2-D cases. It is
found that high degrees of localization in reduced dimensionalities bring about the possibility that, in spite of a weak polaronic coupling, the polaron problem may exhibit a pseudo strong-coupling counterpart coming from the confinement effect.

Table 1.1: Scaling relation between certain quantities : The binding energy E_p, the polaron mass (m_p), and the mean number of phonons, N_{ph} . The upper (lower) row corresponds to the 3D (2D) cases.

	E_p	m_p	N_{ph}
Weak Coupling	$\frac{p}{2}a$ a	$\frac{p}{6}a$ $\frac{1}{6}a$	$\frac{p}{4}a$ $\frac{1}{2}a$
Strong coupling	$\frac{p}{8}a^2$ $\frac{1}{3p^2}a^2$	$\frac{p^2}{16}a^2$ $\frac{16}{81p^2}a^2$	$\frac{p}{4}a^2$ $\frac{2}{3p}a^2$

The study of bound polaron is of interset for a better understanding of centers consisting of an electron bound to a charged impurity or a vacancy in a polar semiconductor or an ionic crystal. For example, the spectra of shollow impurities in polar semiconductors are influenced by the Fröhlich interaction. The bound polaron is also of some interset to the exciton problem as a limiting case where one of the masses tends to the infinity.

The conclusion from these studies [18,19] is that the coulomb interaction exhances the electron-phonon interaction significantly. Furthermore, these effects grow at a much faster rate in 2D then in 3D.

When the strength of the polaronic coupling and the coulomb potential are increased. In a previous work[18,19]we have study the ground state and the first two excited states for a bound polaron in the absence of the magnetic field.

The problem of a polaron in a magnetic field plays an important role in conferming the effect of the confinement in enhancing the polaronic aspect. It has been observed that for strong magnetic fields the phonon part of the ground state energy in 2D grows at the rate $\sqrt{b}$ which is much faster than in 3D where the magnetic dependence is $\ln b$ (Coulomb strength).

The problem of a polaron in a magnetic field has received extensive treatment[20]. Larsen [21] used a variational method closely related to the intermediate coupling method of Lee, Low, and Pines to calculate the ground state energy and the low-lying excited states of the Fröhlich Hamiltonian with a uniform time independent magnetic field. In 1970, Porsch, [22] has calculated the ground state energy in a magnetic field of arbitrary strength in the strong-coupling regime and approximate analytical formula was given in the weak and strong magnetic field cases.

An important comment about the strong-coupling treatment of a polaron in a strong magnetic field is that the adiabatic theory does not give the right weak polaronic coupling limit. This has been corrected by making the lattices displacement centered on the center of the orbit rather than on the average electron position. This modified approach also gives better results for the strong polaronic coupling [23]. Using the same theory Ercelebi et al [24] reconsider the magnetopolaron problem but with a variational technique that interpote the weak and the strong coupling aspect of the problem via variational trial function.

1.4 The Objective of the Study

In this work we retreive the problem of a bound polaron under the effect of an external magnetic field. The energy of the ground state and the first two excited states are calculated using the strong-coupling approach. We also calculated the number of phonons around the electron and the radius of the polaron for the three states. All the above quantities are calculated with and without the magnetic field.

In chapter 1, named as Introduction we introduced the concept of the polaron and gave a survey of the different theories used to solve the problem. Chapter 2, is devoted to the theory with all the analytical calculation. The last chapter contains the results and discussion with conclusion remarks at the end of the chapter.

Chapter 2

Theory

2.1 The Hamiltonian

In the frame work of the adiabatic approximation, the Hamiltonian of a two dimensional electron immersed in the field of bulk (LO) phonon, using the phonon energy $\hbar w_{LO}$ as a unit of energy and $\sqrt{\frac{\hbar}{2m w_{LO}}}$ the polaron radius as a unit of length, with *m* is the effective mass of the electron, is given by [25].

$$H = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q \Gamma_Q \left\{ a_Q \exp(i\vec{q}\cdot\vec{r}) + a_Q^\dagger \exp(-i\vec{q}\cdot\vec{r}) \right\} \quad (2.1)$$

Where H_e is the electronic part of the Hamiltonian, the second term represents the phonon part with a_Q and $a_Q^\dagger$ are the annihilation and creation operators of a phonon of wave vector $\vec{Q} = q + q_z k$ and frequencey w_{LO} and the last term is the electron phonon interaction.

The electron-phonon interaction amplitude is:

$$\Gamma_Q = \sqrt{\frac{4pa}{V}} Q^{-1} \tag{2.2}$$

,V is the volume and a is the electron-phonon coupling constant.

For an electron bound to the hydrogenic impurity ,the electronic part of the Hamiltonian in cylindrical coordinates is,

$$H_e = -\frac{P^2}{2m} - \frac{b}{r} = -\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial f^2} - \frac{\partial^2}{\partial z^2} - \frac{b}{r} \tag{2.3}$$

The dimensionless parameter $b = \left(\frac{e^2}{\varepsilon_o}\right)\sqrt{\frac{2m}{\hbar^3 w_{LO}}}$ stands for the strength of the Coulomb potential .(e is the charge of the electron and ε_o is the permittivity of free space).

To solve the above defined Hamiltonian in the frame work of the strong coupling, we take the pekar (1954) – type trial ansatz which is separable into the electron part j_e and the phonon part , we choose

$$y = j_e\, e^S \,|0\rangle \tag{2.4}$$

where $|0\rangle$ is the phonon vacuum because at low temperature there will be no effective phonons and e^S is the displaced oscillator with

$$S = \sum_Q \Gamma_Q S_Q \left(a_Q - a_Q^\dagger\right) \tag{2.5}$$

Under this displaced oscillator, the Hamiltonian transforms to the form:

$$H \rightarrow H' = e^{-S} H e^{S} \tag{2.6}$$

So we obtain

$$\begin{aligned} H' &= e^{-s} H_e \, e^{s} + e^{-s}\left(\sum_Q a_Q^\dagger a_Q\right)e^{s} \\ &+ e^{-s}\left(\sum_Q \Gamma_Q a_Q e^{i\vec{q}\cdot\vec{r}}\right)e^{s} + e^{-s}\left(\sum_Q \Gamma_Q a_Q^\dagger e^{-i\vec{q}\cdot\vec{r}}\right)e^{s} \end{aligned} \tag{2.7}$$

Now, using the identity:

$$e^{-A} B e^{A} = B + [B,A] + \frac{1}{2!}\big[[B,A],A\big] + \ldots \tag{2.8}$$

and knowing that H_e commutes with a_Q and $a_Q^\dagger$ we get,

$$e^{-S} H_e e^{S} = H_e \tag{2.9}$$

and

$$e^{-S} a_Q^\dagger a_Q e^{S} = a_Q^\dagger a_Q - \Gamma_Q S_Q \left(a_Q^\dagger + a_Q\right) + \Gamma_Q^2 S_Q{}^2 \tag{2.10}$$

$$e^{-S} a_Q e^{S} = a_Q - \Gamma_Q S_Q \tag{2.11}$$

$$e^{-S} a_Q^\dagger e^{S} = a_Q^\dagger - \Gamma_Q S_Q \tag{2.12}$$

From eqs 2.9 - 2.12 we get,

$$H' = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q \Gamma_Q^2 S_Q{}^2 - \sum_Q \Gamma_Q^2 S_Q (e^{i\vec{q}\cdot\vec{r}} + e^{-i\vec{q}\cdot\vec{r}})$$
$$+ \sum_Q \Gamma_Q \left\{ h_Q a_Q + h^* a_Q{}^\dagger \right\} \tag{2.13}$$

with,

$$h_Q = (e^{i\vec{q}\cdot\vec{r}} - S_Q)$$

By optimizing $\langle j_e | \langle 0 | H' | 0 \rangle | j_e \rangle$ with respect to S_Q we get,

$$S_Q = \langle j_e | e^{\pm i \vec{q}\cdot\vec{r}} | j_e \rangle \tag{2.14}$$

Also for the energy we obtain,

$$E = e_0 - e_p \tag{2.15}$$

where

$$e_0 = \langle \varphi_e | H_e | \varphi_e \rangle \tag{2.16}$$

and

$$e_p = \sum_Q \Gamma_Q^2 S_Q^2 \tag{2.17}$$

The average number N of virtual phonons in the cloud around the electron is calculated by finding the expectation value of the phonon part of the Hamiltonian (the second term of equation 2.1), that is,

$$N = \langle y \,|\sum_Q a_Q^\dagger a_Q\, | y \rangle \tag{2.18}$$

Using the definition of y given in eq(2.4) and the transformation of eq(2.10) we obtain :

$$N = \langle 0|\sum_Q a_Q^\dagger a_Q\,|0\rangle - \Gamma_Q S_Q \,\langle 0|\sum_Q \left(a_Q^\dagger + a_Q\right)|0\rangle + \Gamma_Q^2 S_Q{}^2 \,\langle 0|0\rangle \tag{2.19}$$

which yields

$$N = \sum_Q \Gamma_Q^2 S_Q^2$$

The size of the polaron is the expectation value of the operator r , in other words,

$$R = \left\langle \Phi_e \,\middle|\, r \,\middle|\, \Phi_e \right\rangle \tag{2.20}$$

For the electronic part of the wavefunction we choose the hydrogenic-like behavior and thus use for the ground state and the first two excited states 1s,2s and 2p,the wavefunctions,

$$\Phi_{1s} = \sqrt{\frac{8}{p}}\, s\, e^{-2s\, r} \tag{2.21}$$

$$\Phi_{2s} = \sqrt{\frac{8}{27p}}\left(s - \frac{4s^2}{3} r \right) e^{\frac{-2s}{3} r} \tag{2.22}$$

$$\Phi_{2p} = \frac{8s^2}{9\sqrt{3p}}\, r e^{iq} e^{\frac{-2s}{3} r} \tag{2.23}$$

with σ is a variational parameter.

2.2 The Ground State :

To evaluate e_0 for the ground state Φ_{1s} we have,

$$e_0 = \langle \varphi_{1s} | H_e | \varphi_{1s} \rangle = \int j_{1s}{}^{*} H_e j_{1s} dt$$

$$= \int_0^{2p} \int_0^{\infty} \sqrt{\frac{8}{p}} s e^{-2sr} \left(-\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) - \frac{1}{r^2} \frac{\partial^2}{\partial f^2} - \frac{b}{r} \right) \sqrt{\frac{8}{p}} s e^{-2sr} \, r d r d f$$

$$= 4s^2 - 4bs \qquad (2.24)$$

and to obtain e_p we have,

$$S_Q = \langle j_{1s} | e^{\pm i \vec{q} \cdot \vec{r}} | j_{1s} \rangle = \frac{1}{\left(1 + \frac{q^2}{16 s^2} \right)^{\frac{3}{2}}} \qquad (2.25)$$

$$e_p = \frac{V}{(2p)^3} \int_0^{2p} \int_{-\infty}^{\infty} \frac{4pa}{V} Q^{-2} \frac{1}{\left(1 + \frac{q^2}{16 s^2} \right)^3} q dq dq_z df$$

$$= \frac{3}{4} pas \qquad (2.26)$$

So the ground state energy is given by:

$$E_{1s} = 4s^2 - 4bs - \frac{3}{4} pas \qquad (2.27)$$

The average number of phonons and the radius of the phonons are respectively,

$$N_{1s} = \frac{3}{4} p a s \tag{2.28}$$

and

$$R_{1s} = \frac{1}{2s} \tag{2.29}$$

By minimizing $E = e_0 - e_p$ with respect to σ we get for the ground state energy

$$E_{1s} = -(b + 0.1875 p a)^2 \tag{2.30}$$

and for the average number of phonons around the electron, and the polaron size, in the ground state we obtain, respectively

$$N_{1s} = \frac{3}{4} p a \left(\frac{b}{2} + 0.0937 p a \right) \tag{2.31}$$

$$R_{1s} = (b + 0.1875 p a)^{-1} \tag{2.32}$$

2.3 The First Excited State:

To evaluate e_0 for the first excited state Φ_{2s}, we have

$$e_0 = \langle \varphi_{2s} | H_e | \varphi_{2s} \rangle = \int j_{2s} H_e j_{2s}^{*} dt$$

Then,

$$e_0 = \int_0^{2p}\int_0^{\infty}\sqrt{\frac{8}{27p}}\left(s - \frac{4s^2}{3}r\right)e^{-\frac{2s}{3}r}\left(-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial f^2} - \frac{b}{r}\right)$$
$$\sqrt{\frac{8}{27p}}\left(s - \frac{4s^2}{3}r\right)e^{\frac{-2s}{3}r}\, rdrdf$$

$$= \frac{4}{9}s^2 - \frac{4}{9}bs \qquad (2.33)$$

and to obtain e_p we have,

$$S_Q = \langle j_{2s}|e^{\pm i\vec{q}\cdot\vec{r}}|j_{2s}\rangle = m^{-3} - 5m^{-5} + 5m^{-7}$$

Where, $\qquad m = \sqrt{1 + \left(\frac{3q}{4s}\right)^2}$

$$e_p = \frac{V}{(2p)^3}\int_0^{2p}\int_0^{\infty}\frac{4pa}{V}Q^{-2}\left(m^{-3} - 5m^{-5} + 5m^{-7}\right)^2 qdqdq_z df$$

$$= \left(\frac{53}{512}\right)pas \qquad (2.34)$$

So the first excited state energy becomes

$$E_{2s} = \frac{4}{9}s^2 - \frac{4}{9}bs - \frac{53}{512}pas \qquad (2.35)$$

For the number of phonons and the size of the polaron we have,

$$N_{2s} = \left(\frac{53}{512}\right) p a s \tag{2.36}$$

and,

$$R_{2s} = \frac{7}{2s} \tag{2.37}$$

Minimizing Eq.2.35 with respect to σ we obtain for the first excited state energy

$$E_{2s} = -\left(\frac{b}{3} + 0.0776 p a\right)^2 \tag{2.38}$$

The average number of phonons around the electron and the polaron size in the first excited state are, respectively

$$N_{2s} = 0.104 p a \left(\frac{b}{2} + 0.1160 p a\right) \qquad , \tag{2.39}$$

$$R_{2s} = 7\left(b + 0.2330 p a\right)^{-1} \tag{2.40}$$

2.4 The Second Excited State:

To evaluate e_0 for the second excited state Φ_{2p}, we have

$$e_0 = \left\langle \varphi_{2p} \middle| H_e \middle| \varphi_{2p} \right\rangle = \int j_{2p}{}^{*} H_e j_{2p} dt \ ,$$

then,

$$e_0 = \int_0^{2p}\int_0^{\infty} \frac{8s^2}{9\sqrt{3p}} re^{iq} e^{-\frac{2s}{3}r} \left(-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial f^2} - \frac{b}{r}\right)$$
$$\frac{8s^2}{9\sqrt{3p}} e^{iq} e^{-\frac{2s}{3}r} \, r\,d\,r\,d\,f$$

$$= \frac{4}{9}s^2 - \frac{4}{9}bs \tag{2.41}$$

and to obtain e_p we have,

$$S_Q = \left\langle j_{2p} \left| e^{\pm i\vec{q}\cdot\vec{r}} \right| j_{2p} \right\rangle = \frac{5}{2}m^{-7} - \frac{3}{2}m^{-5}$$

$$e_p = \frac{V}{(2p)^3}\int_0^{2p}\int_{-\infty}^{\infty} \frac{4pa}{V} Q^{-2}\left(\frac{5}{2}m^{-7} - \frac{3}{2}m^{-5}\right)^2 qdqdq_z df$$

$$= \left(\frac{245}{2^{11}}\right) pas \tag{2.42}$$

From eqs. 2.41 and 2.42 we get,

$$E_{2p} = \frac{4}{9}s^2 - \frac{4}{9}bs - \frac{245}{2^{11}}pas \tag{2.43}$$

For the number of phonons and the size of the polaron we have,

$$N_{2p} = \left(\frac{245}{2^{11}}\right) pas \tag{2.44}$$

and

$$R_{2p} = \frac{3}{s} \tag{2.45}$$

Again minimizing equ. 2.43 with respect to σ we obtain

$$E_{2p} = -\left(\frac{b}{3} + 0.0897pa\right)^2 \quad , \tag{2.46}$$

$$N_{2p} = 0.120pa\left(\frac{b}{2} + 0.1350pa\right) \quad , \tag{2.47}$$

$$R_{2p} = 6(b + 0.2690pa)^{-1} \quad . \tag{2.48}$$

2.5 The effect of magnetic field

The application of an external magnetic field on the polaron puts a further confinement on the problem making the electron-phonon interaction more pronounced. A part from the competition between the magnetic and the Coulomb fields, the polaronic effect introduce further complications. Reasonable simplifications however can be achieved on the extreme limits of the magnetic field. For sufficiently high magnetic fields, the lattice can only respond to the mean charge density of the rapidly orbiting electron and hence acquire a static deformation over the entire Landau orbit (Ercelebi and Saqqa)[24]. Thus the most efficient coherent phonon state should be taken as centerd on the orbit center rather than on the origin as assumed by adopting the displaced oscillator defined in (Eq.2.5). For not too large magnetic magnetic fields and strong phonon coupling, the polaronic aspect dominates the magnetic field counterpared of the problem so that the lattice deformation should be thought as surrounding the mean charge density of the electron itself rather than it overall motion in a Landau orbit.

An important contributions to the theoretical study of polarons in magnetic fields was made by Larsen [9]. In particular he was the first to point out the level repulsion close to the crossing of levels at ($\Omega = w_{LO}$ is strength of magnetic field).

Using the symmetric guage $\vec{A} = \frac{B}{2}(-y, x, 0)$ for the vector potential, the electronic part of the Hamiltonian of a two dimensional polaron immeresed in a magnetic field $\vec{B} = B\hat{Z}$ is :

$$H_e = \frac{P^2}{2m} - \frac{b}{r} + \frac{1}{16}\Omega^2 r^2 + \frac{1}{2}L_Z\Omega \tag{2.49}$$

Where $\vec{r} = (x, y)$ denotes the electron position in the transverse plane, $\left(L_Z = xP_y - yP_x\right)$ is the angular momentum, and $\Omega = \frac{eB}{mcw_{LO}}$ is the dimensionless cyclotron frequencey.

Using cylindrical coordinates, the electronic Hamiltonian becomes:

$$H_e = -\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial f^2} - \frac{\partial^2}{\partial z^2} - \frac{b}{r} + \frac{1}{16}\Omega^2 r^2 - i\hbar\left(\frac{\Omega}{2}\right)\frac{\partial}{\partial f} \tag{2.50}$$

The expectation value under the same wave functions defined by equation (2.15) is :

$$\langle j_e | \langle 0 | H' | 0 \rangle | j_e \rangle = E = e_0 - e_p \tag{2.51}$$

But now,

$$e_0 = \langle \varphi_e | H_e | \varphi_e \rangle = \int j_e^* H_e j_e dt$$

$$= \langle \Phi_e | P^2 - \frac{b}{r} | \Phi_e \rangle + \langle \Phi_e | \frac{1}{16} \Omega^2 r^2 | \Phi_e \rangle + \frac{1}{2} \Omega \langle \Phi_e | L_Z | \Phi_e \rangle \tag{2.52}$$

For the ground state we have,

$$e_0 = \langle \Phi_e | P^2 - \frac{b}{r} | \Phi_e \rangle = 4s^2 - 4bs \tag{2.53}$$

$$e_p = \frac{3}{4} pas \tag{2.54}$$

$$\langle \Phi_e | \frac{1}{16} \Omega^2 r^2 | \Phi_e \rangle = \frac{3}{128} \frac{\Omega^2}{s^2} \tag{2.55}$$

and because Φ_{1s} does not depend on f, we get

$$\frac{1}{2} \Omega \langle \Phi_e | L_Z | \Phi_e \rangle = -i \frac{\hbar}{2} \Omega \langle \Phi_e | \frac{\partial}{\partial f} | \Phi_e \rangle = 0 \tag{2.56}$$

From these equations we get

$$E_{1s} = 4s^2 - 4bs - \frac{3}{4} pas + \frac{3}{128} \frac{\Omega^2}{s^2} \tag{2.57}$$

and for the first excited state,we obtain:

$$e_0 = \frac{4}{9}s^2 - \frac{4}{9}bs \qquad , \tag{2.58}$$

$$e_p = \left(\frac{53}{512}\right)pas \quad , \tag{2.59}$$

$$\left\langle \Phi_e \left| \frac{1}{16}\Omega^2 r^2 \right| \Phi_e \right\rangle = \frac{117}{128}\frac{\Omega^2}{s^2} \quad , \tag{2.60}$$

and, again since Φ_{2s} does not depend on f ,

$$\frac{1}{2}\Omega\left\langle \Phi_e \left| L_Z \right| \Phi_e \right\rangle = -i\frac{\mathbf{h}}{2}\Omega\left\langle \Phi_e \left| \frac{\partial}{\partial f} \right| \Phi_e \right\rangle = 0 \tag{2.61}$$

These lead to

$$E_{2s} = \frac{4}{9}s^2 - \frac{4}{9}bs - \frac{53}{512}pas + \frac{117}{128}\frac{\Omega^2}{s^2} \tag{2.62}$$

Now for the second excited state, we have

$$e_0 = \frac{4}{9}s^2 - \frac{4}{9}bs \tag{2.63}$$

$$e_p = \left(\frac{245}{2^{11}}\right)pas \tag{2.64}$$

$$\left\langle \Phi_e \left| \frac{1}{16}\Omega^2 r^2 \right| \Phi_e \right\rangle = \frac{45}{64}\frac{\Omega^2}{s^2} \tag{2.65}$$

and,

$$\frac{1}{2}\Omega\left\langle \Phi_e \left| L_Z \right| \Phi_e \right\rangle = -i\frac{\mathbf{h}}{2}\Omega\left\langle \Phi_e \left| \frac{\partial}{\partial f} \right| \Phi_e \right\rangle = 0 \tag{2.66}$$

Combining these equations we have

$$E_{2p} = \frac{4}{9}s^2 - \frac{4}{9}bs - \frac{245}{2^{11}}pas + \frac{45}{64}\frac{\Omega^2}{s^2} \qquad (2.67)$$

Note that the formulas that gives the number of phonons and the size of the polaron will not be changed quantitavely. The application of the magnetic field will affect these two values implicitely through the variational parameter σ .

Chapter 3

Results and Discussion

Before we present our results concerning the coupled effect of both the electron-phonon interaction and the magnetic field on the problem, we would like to discuss some special cases where the situation is more clear and well-known. For the bare two-dimensional polaron ($\beta=\Omega=0$) we get $E=-0.347\alpha^2$ which differ from the standard strong coupling value given in table (1.1) by about 11% . The discrepancy here is due to the wave function adopted. The Hydrogen-like wave function used in this work is suitable only for bound problem and so for $\beta=0$, the Gaussian wave function is supposed to be more appropriate.

Without the polaronic effect and in the absence of the magnetic field ($\alpha=0,\Omega=0$) we trivially obtain $E=-\beta^2$ which is the 2D-Rydberg which is four times that for the 3D case.

For the bare donor in a magnetic field ($\alpha=0$) we refere to the paper by MacDonald and Recheie[26]. In the high magnetic field limit they obtain :

$$E = 2b^2 g \left(0.5 - c - 0.04401c^2 - 0.02331c^3 - 0.00727c^4 ....\right)$$

where,

$$c = \sqrt{\frac{p}{8g}} \quad \text{and} \quad g = \frac{\Omega}{2b^2} \ ,$$

is a measure of the strength of the magnetic field relative to the 2D-effective Rydberg, β^2 and for weak magnetic field $\gamma \leq 0.1$ they obtain $E = -b^2\left(1 - \frac{3}{8}g^2\right)$. In table 3.1 we tabulate our results with that for $\Omega=0.1$. As it is clear from the table the agreement is exact between the two results for $\Omega > \beta$. The discrepencey between the two results comes from the choice of the wave function. For $\Omega > \beta$ the H-like wave function lose its validity.

Table 3.1 ($\alpha=0$).

β	$\beta=0.1$	$\beta=0.5$	$\beta=1.0$	$\beta=5.0$
E_{1s}	0.02333	-0.2463	-0.99906	-25.00
E_M	0.08375	-0.2463	-0.99906	-25.00
E_{1s}(Present work)	0.02332	-0.2463	-0.99906	-25.00

Taking the remaining case ($\beta=0$) the problem reduces to the 2D, magnetopolaron which was studied in detail by Ercelebi and Saqqa[24].

We now turn back to the donor problem and study the polaronic effect together with the additional enhancement coming from the magnetic field on the ground state and the first two excited state. To show the effect of the electron-phonon coupling on the problem we plot in Figure 3.1 the ground state energy as a function of the coupling constant α for two values of the

Coulomb field strength (β=1 and β=10). We at once notice that the effect of the polaronic interaction on the binding energy becomes more pronounced as β is increased. To show this phenomena in more details we display in Figure 3.2 the average number of phonons in the cloud surrounding the electron in the ground state as a function of α for the same values of β.

Again the figure tells that the polaronic effect becomes more important as the Coulomb field increases. The reason for this feature is explained as follow: As β is increased, the binding energy becomes deeper making the localization of the electron more pronounced and this, in turn, increases the importance of the polaronic correction. In Figure 3.3 we plot the polaron size in the ground state energy as a function of α for β=1 and β=10 as before. We note that the α-dependence on the polaron size becomes more prominent as β gets smaller.

In Figure 3.4 we display the energies of the two excited states as a function of α for β=1 and β=10. As it is clear from the graph, the polaronic effect lifts the degeneracy of the two states. The degeneracy is removed at lower values of α as β is increased and this support the phenomena discussed previously. The Coulomb field strength enhances the importance of the polaronic effect.

To show the effect of the external magnetic field on the problem we plot in Figure 3.5 the ground state energy as a function of the strength of the magnetic field for two different values of the coulomb strength. As it is clear from the graph, the importance of the Coulomb strength becomes more important as Ω is increased. Morever, the effect of the magnetic field on the energy is more clear for larger values of β. The reason behind this feature is that the strength of the three fields, (the polaronic, the Coulomb and the magnetic field) do not enter the problem independently, but affect the contributions one another in a somewhat involved and interrelated manner. The same feature shows up in Figure 3.6 where we plot the two excited states as a function of Ω for the same values of β.

In Figure 3.7 and Figure 3.8 we plot, respectively the number of phonons and the polaron size in the ground state versus Ω again for β=1 and β=10.

For a given value of Ω, the bound polaron cloud appears to contains a smaller number of phonons when β=1 than β=10. The Ω-dependence in the size of the polaron becomes more prominant as β gets smaller.

In Figure 3.9 and Figure 3.10 we display the effect of the magnetic field on the number of phonons and the size of polarons, respectively for the two excited states. The polaron size in the excited states exhibits qualitatively the same behavior as the ground state. For large value of β we note that the size does not change appreciably over a wide range of Ω. The effect of the magnetic field on the number of phonons is more solid for β=10.

It should be noted that for too large values of the magnetic field, the coherent state we adopt in this work may be not fit to reflect a correct description of the problem, specially for smaller values of the polaronic constant α . In this limit the lattice can only respond to the mean charge density of the rapidly orbiting electron and hence acquire a static deformation over the entire Landau orbit rather than about the origin.

Conclusion:

In this work we have retreived the problem of a two dimensional bound polaron using the strong coupling approach. The energy of the first three-levels has been calculated in addition to the average number of phonons around the electron and the size of the polaron in the three states. It is found that the polaronic effect becomes more important as the Coulomb field increases. The degeneracy of the two excited states is observed to be lifted at tower values of the polaronic constant α as the Coulomb constant β decreases.

The effect of an external magnetic field on the problem is also studied. The strength of the three fields: the polaronic field, the Coulomb field and the magnetic field do not enter the problem independently but rather affect each other in an involved and inetrrelated manner.

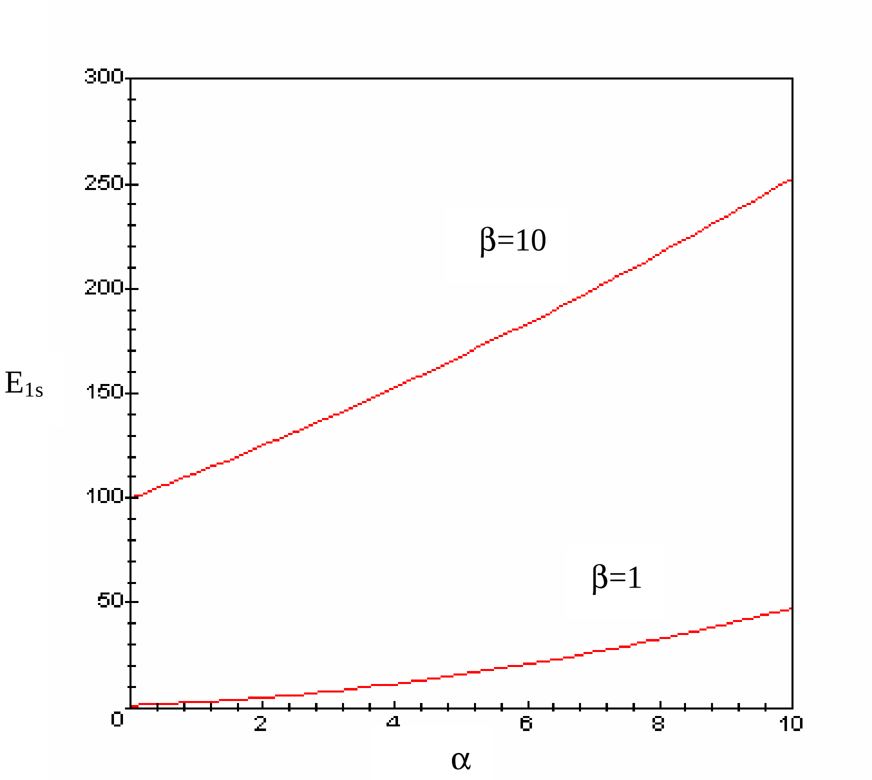

Fig.3.1 The ground state energy E_{1s} in $\hbar w$ as a function of α for β=1 and β=10 and Ω=0.

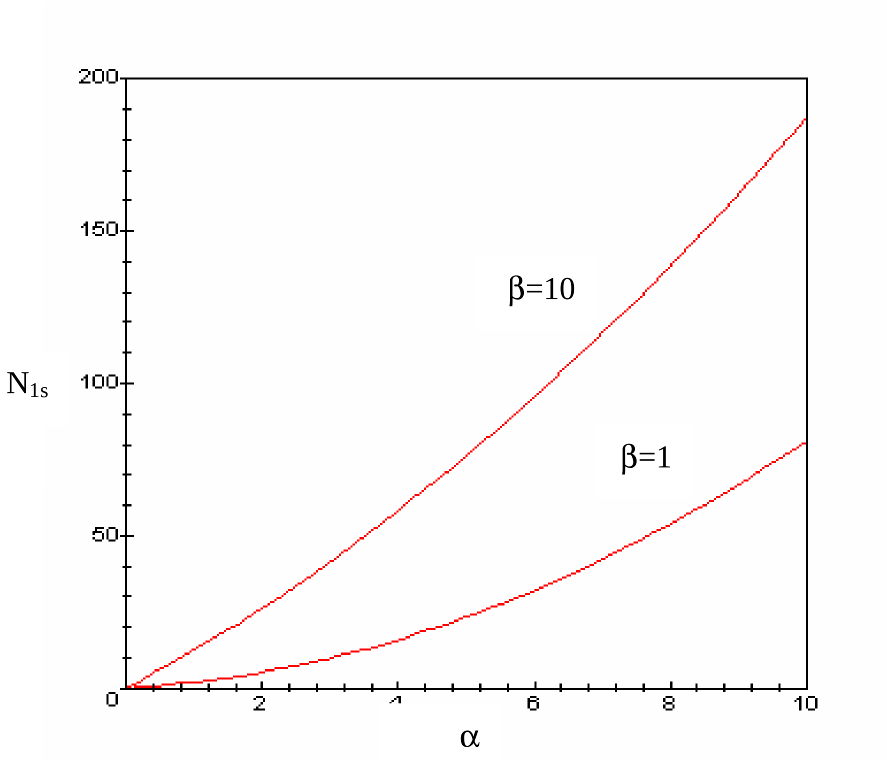

Fig.3.2 The average number of phonons around the electron in the ground state as a function of α for β=1 and β=10 and Ω=0.

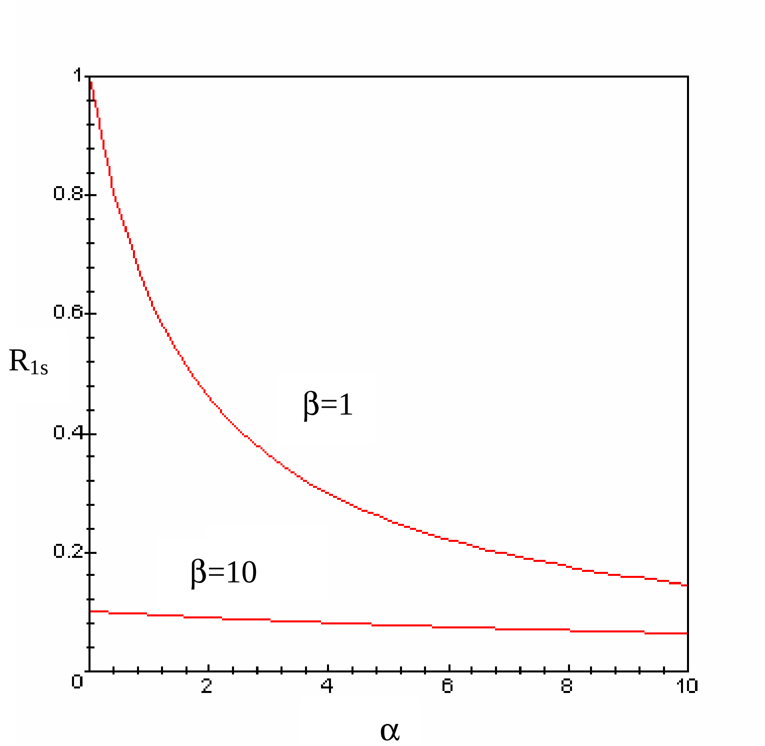

Fig.3.3 The size of the polaron in the ground state as a function of α for β=1 and β=10 and Ω=0.

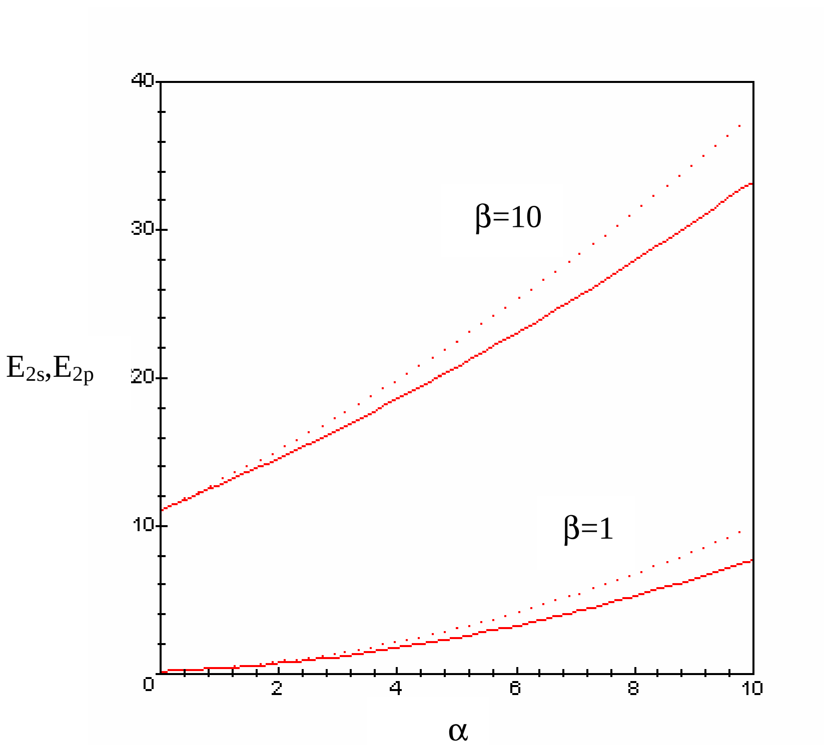

Fig.3.4. The excited state energies in **h***w* as a function of α for β=1 and β=10 and Ω=0. The dashed and the solid curves correspond to the 2s and 2p states respectively.

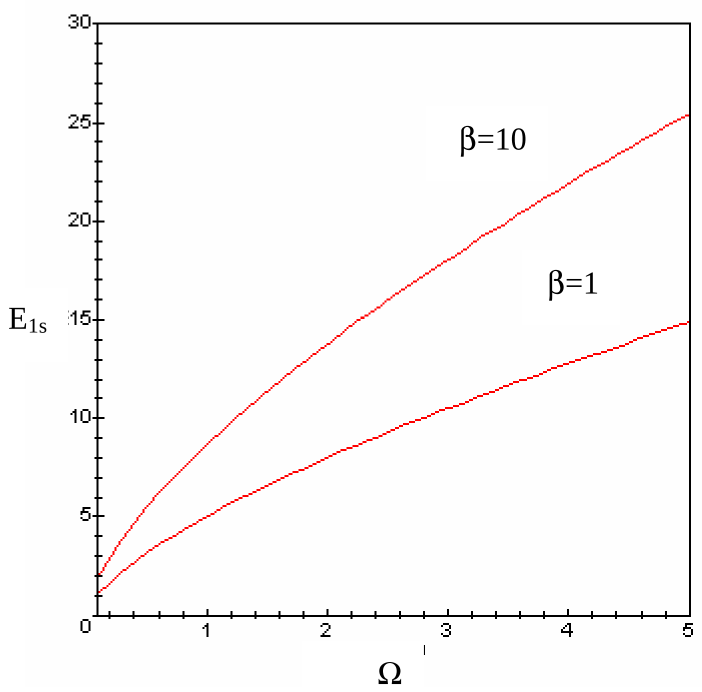

Fig.3.5. The ground state energy in $\hbar w$ (in the presence of magnetic field) as a function of Ω for β=1 and β=10 and α=10.

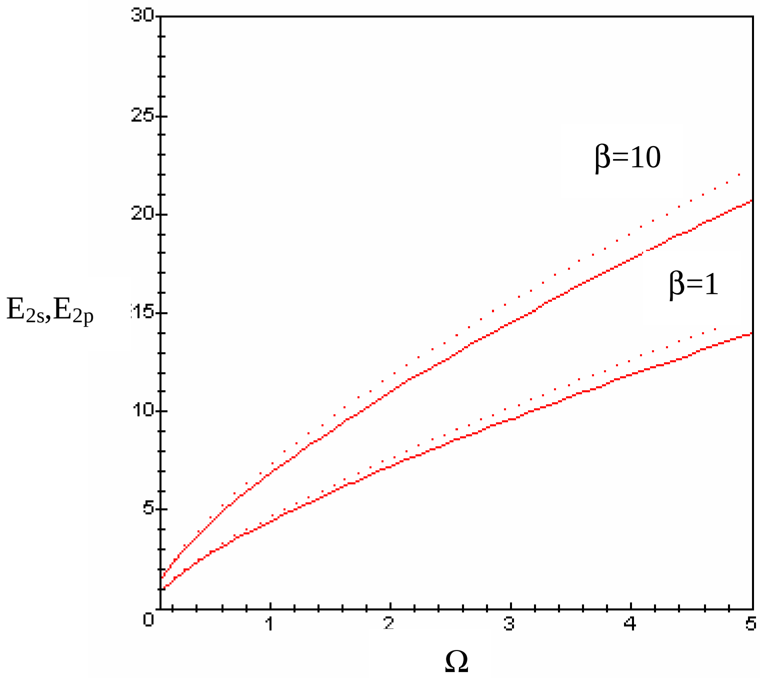

Fig.3.6. The excited energies in $\hbar w$ (in the presence of magnetic field) as a function of Ω for β=1 and β=10 and α=10. The dashed and the solid curves correspond to the 2s and 2p states respectively.

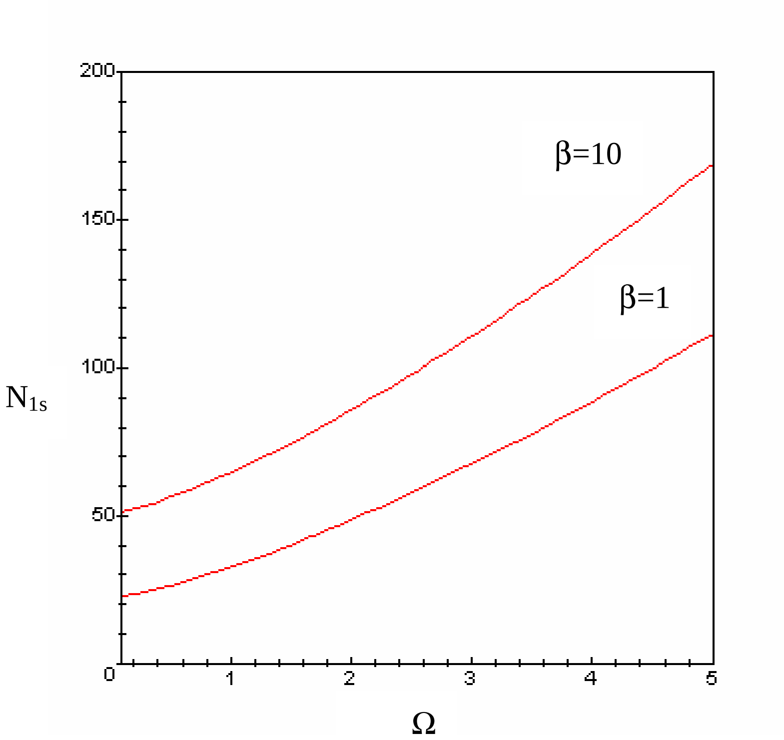

Fig.3.7. The average number of phonons (in the presence of magnetic field) around the electron in the ground state as a function of Ω for β=1 and β=10 and α=10.

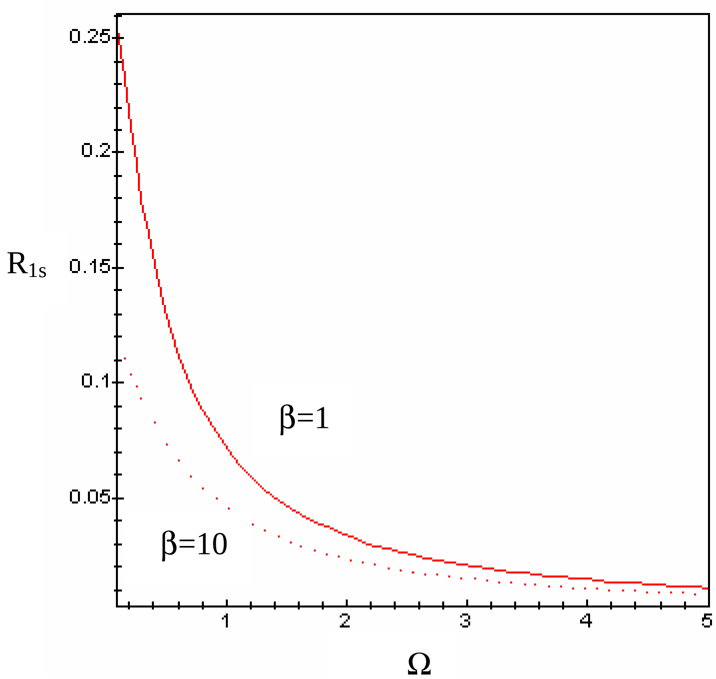

Fig.3.8. The size of the polaron (in the presence of magnetic field) in the ground state as a function of Ω for β=1 and β=10 and α=10.

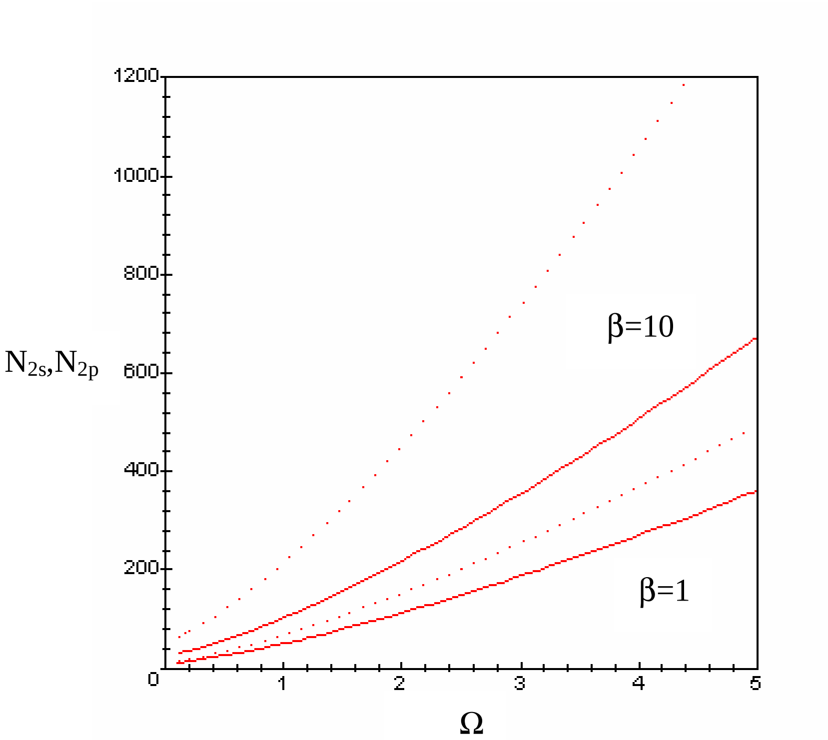

Fig.3.9. The average number of phonons (in the presence of magnetic field) around the electron in the (2s and 2p) states as a function of Ω for β=1 and β=10 and α=10.

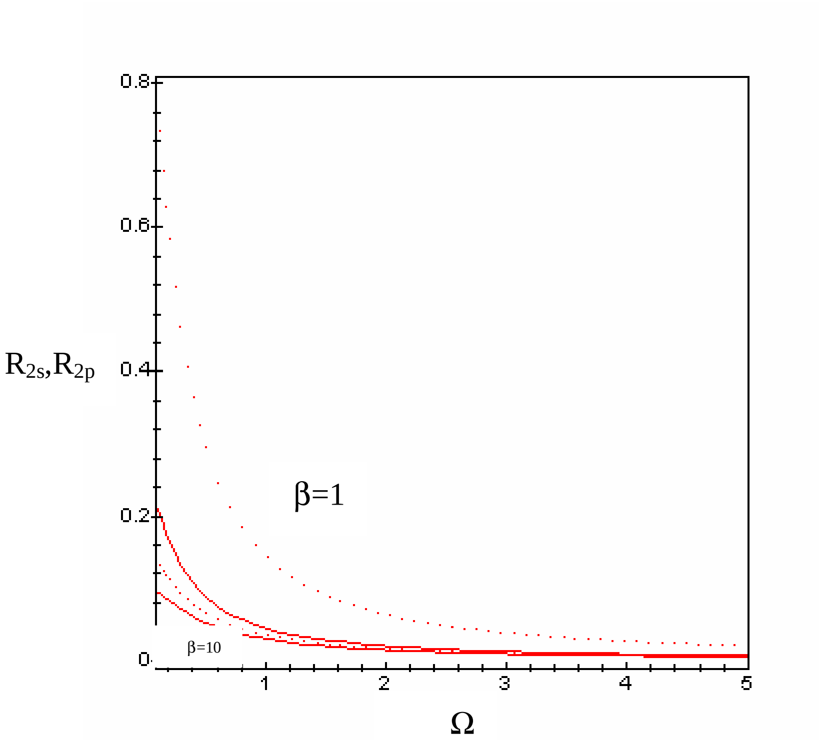

Fig.3.10. The size of polaron (in the presence of magnetic field) in the (2s and 2p) states as a function of Ω for β=1 and β=10 and α=10.

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